

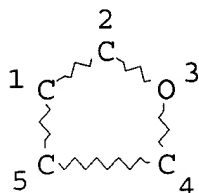
B. Dentz Oct 31, 1955

S.N. 08/425022 applicant
Bertenshaw

=> stru

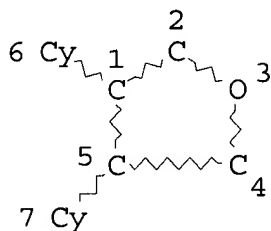
ENTER NAME OF STRUCTURE TO BE RECALLED (NONE):.

ENTER (DIS), GRA, NOD, BON OR ?:gra r5,nod 3 o,dis

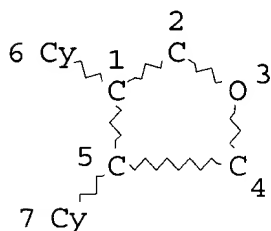


search for ~~X~~ gets.
wherein X is H

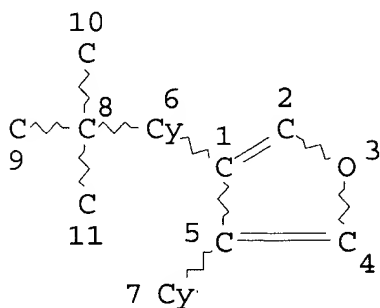
ENTER (DIS), GRA, NOD, BON OR ?:gra 1 c1,5 c1,nod 6 7 cy,dis



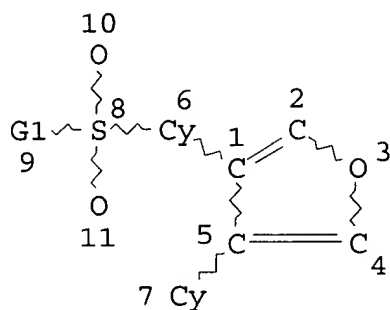
ENTER (DIS), GRA, NOD, BON OR ?:ggc 6 7 uns,dis



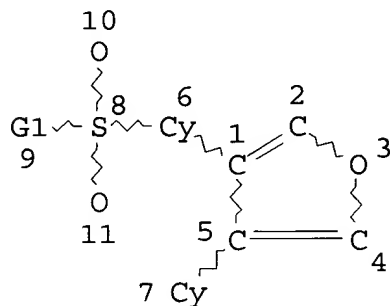
ENTER (DIS), GRA, NOD, BON OR ?:bon 1-2 4-5 de,gra 6 c2,8 c1,8
c1,dis



ENTER (DIS), GRA, NOD, BON OR ?:nod 8 s,10 11 o,9 g1,var
g1=c/n,dis



VAR G1=C/N
ENTER (DIS), GRA, NOD, BON OR ?:rsp,dis sia



VAR G1=C/N
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 6
GGCAT IS UNS AT 7
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE
ENTER (DIS), GRA, NOD, BON OR ?:end
L1 STRUCTURE CREATED

=>
=> s 11
SAMPLE SEARCH INITIATED 11:10:58
SAMPLE SCREEN SEARCH COMPLETED - 898 TO ITERATE
100.0% PROCESSED 898 ITERATIONS
ANSWERS
SEARCH TIME: 00.00.21

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 16164 TO 19756

PROJECTED ANSWERS:

0 TO

0

L2 0 SEA SSS SAM L1

=> s l1 ful

FULL SEARCH INITIATED 11:12:32

SCREENING

SCREENING

SCREENING

FULL SCREEN SEARCH COMPLETED - 17680 TO ITERATE

66.1% PROCESSED 11681 ITERATIONS 1

ANSWERS

96.7% PROCESSED 17100 ITERATIONS 1

ANSWERS

99.5% PROCESSED 17593 ITERATIONS 1

ANSWERS

100.0% PROCESSED 17680 ITERATIONS 1

ANSWERS

SEARCH TIME: 00.01.48

L3 1 SEA SSS FUL L1

=> d sub bib abs

L3 ANSWER 1 OF 1 REGISTRY COPYRIGHT 1995 ACS

RN 157671-80-2 REGISTRY

CN Furan, 3-(4-fluorophenyl)-4-[4-(methylsulfonyl)phenyl] -
(9CI) (CA

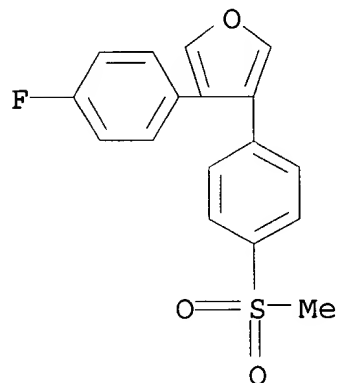
INDEX NAME)

FS 3D CONCORD

MF C17 H13 F O3 S

SR CA

LC STN Files: CA, CAPLUS, CAPREVIEWS



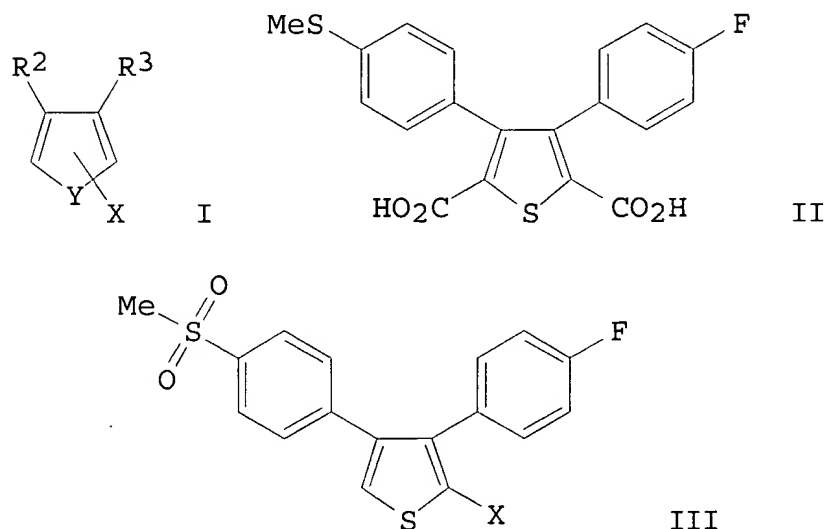
1 REFERENCES IN FILE CAPREVIEWS

1 REFERENCES IN FILE CA (1967 TO DATE)

2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1

AN 121:179484 CA
 TI Novel 3,4-diaryl thiophenes and analogs thereof having use
 as antiinflammatory agents
 IN Bertenshaw, Stephen R.; Collins, Paul W.; Penning, Thomas
 D.; Reitz,
 David B.; Rogers, Roland S.
 PA Searle, G. D., and Co., USA
 SO PCT Int. Appl., 96 pp.
 CODEN: PIXXD2
 PI WO 9415932 A1 940721
 DS W: AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, ES, FI,
 GB, HU,
 JP, KP, KR, KZ, LK, LU, LV, MG, MN, MW, NL, NO, NZ, PL,
 PT, RO,
 RU, SD, SE, SK, UA, US, UZ, VN
 RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB,
 GR, IE,
 IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG
 AI WO 94-US466 940114
 PRAI US 93-4822 930115
 DT Patent
 LA English
 GI



AB A class of 3,4-diaryl-substituted thiophene, furan, and
 pyrrole
 derivs. is disclosed, as well as pharmaceutical compns.
 contg. them,

and methods of using them to treat inflammation and related disorders. Compds. of particular interest are I [Y = S, O, NR1; R1

= H, lower alkyl; X = 1 or 2 substituents selected from a large

group, esp. H, halo, lower alkoxy carbonyl, CO₂H; R₂, R₃ = (independently) aryl or heteroaryl, optionally substituted with 1 or

more radicals such as sulfamyl, alkylsulfonyl, halo, lower alkoxy

and lower alkyl] and pharmaceutically acceptable salts thereof. For

example, S(CH₂CO₂Me)₂ was cyclized with 4-FC₆H₄COCOC₆H₄(SMe)-4 in

THF-MeOH contg. NaOMe at 65.degree. to give 82% of a mixt. of

regioisomeric thiophenedicarboxylic acid monoesters, which were

saponified by NaOH in aq. THF-MeOH to give diacid II. Double decarboxylation of II with Cu in quinoline at 180-200.degree. (89%)

and S-oxidn. with MCPBA gave title compd. III (X = H), which was

brominated by Br₂ in AcOH to give III (X = Br) plus the corresponding 2,5-dibromo compd. III (X = Br) at 10 mg/kg orally

gave 30% inhibition in the carrageenan-induced rat-paw edema test.

Data include 15 synthetic examples, rat-paw edema and analgesia

tests, and in vitro tests for cyclooxygenase (I and II) and TXB₂

activity.